PFHxS

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 235 °C

Global applicability domain: Outside

Local applicability domain index: 3.57e-01

Confidence level: 6.99e-01

Nearest Neighbors from the Training Set

Image not found
PFHxS
Measured: 239
Predicted: 235

Image not found
1-Pentanesulfonic acid,
1,1,2,2,3,3,4,4,5,5,5-
undecafluoro-
Measured: 225
Predicted: 223

Image not found
1-Perfluorobutanesulfonic acid
Measured: 211
Predicted: 212

Image not found
Sulfluramid
Measured: 196
Predicted: 198

Image not found
Heptanoic acid,
2,2,3,3,4,4,5,5,6,6,7,7-
dodecafluoro-
Measured: 192
Predicted: 186